Abstract No. Igar0348

Phase Transition Related to Octahedral Rotation in Sr_2CuWO_6

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Beamline(s): X7A

Introduction: Sr_2CuWO_6 has been known for a long time to undergo a strong first order tetragonal-to-cubic phase transition at about 1190 K [1]. This phase transition is due to the presence of the Jahn-Teller active ion Cu^{2+}. The characteristic feature of the transition is the strong distortion of the CuO_6 octahedra along the tetragonal c-axis. The room temperature structure of Sr_2CuWO_6 was found to be I4/m [2,3]. In this structure the CuO_6 octahedra are not only elongated (which should lead to the I4/mmm space group), but also are rotated, ≈9°, around the same c-axis. The explanation for this rotation cannot be based only on the Jahn-Teller effect, and should also involve another mechanism. Phase transitions related to octahedral tilts and rotations have been observed in many double perovskite compounds. In order to determine whether such a transition also occurs in Sr_2CuWO_6 high-resolution temperature-dependent X-ray diffraction measurements were necessary.

Methods and Materials: Powder sample of Sr_2CuWO_6 was prepared by solid-state method from high purity oxides. X-ray diffraction data were obtained at NSLS X7A beamline using the position sensitive detector. A Si(111) monochromator crystal was used and the wavelength of 0.79997Å was calibrated using a CeO_2 standard. The sample was placed in a quartz capillary and rotated during the experiment.

Results: In our study of the temperature behavior of the structure of Sr_2CuWO_6 with X-ray powder diffraction method, we found evidence of another, very weak, phase transition at about 760 K. The change of the lattice parameters with the temperature is shown in Fig.1. The anomalous behavior around this temperature could be attributed to the presence of a phase transition. This transition is continuous and changes the symmetry from I4/m to another body-centered tetragonal space group. Although no reliable structural determination at this temperature could be performed, the behavior of some diffraction peaks (Fig.2), sensitive to octahedral rotations, points to a possible I4/mmm structure. The I4/mmm—I4/m phase transition is allowed by the Landau theory to be continuous. The mechanism of this transition is of the same type as that of Fm-3m —I4/m, found in many ordered double perovskites and is related to the bond-stress relaxation, due to the mismatch between the size of the Sr cation and the cuboctahedral space between the CuO_6 and WO_6 octahedra.

Conclusions: We suggest that the symmetry lowering from Fm3m to I4/m in Sr_2CuWO_6 is performed in two steps:Fm-3m —1190 K—I4/mmm—760 K—I4/m, and not just in one, as previously reported [3]. We consider two independent phase transition mechanisms, which could explain the structural behavior of Sr_2CuWO_6.

Acknowledgments: This work was supported by the Euskal Herriko Unibertsitatea under project No. UPV0063.310-13564/2001. Authors thank Dr. B. Noheda and Dr. T. Vogt for their help.

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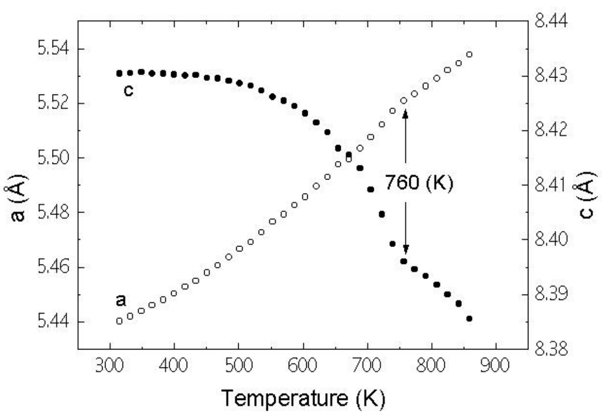

Figure 1. Change of the lattice parameters with the temperature.

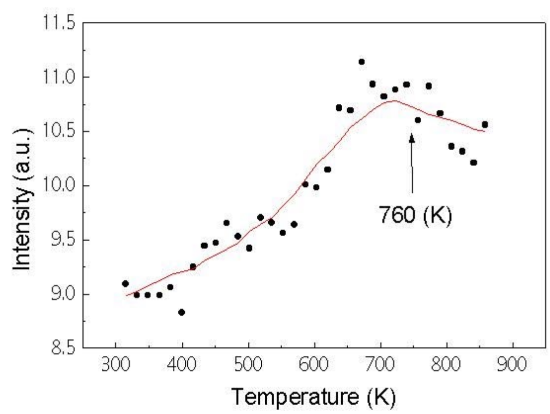

Figure 2. Intensity of the (222) peak. Points represent experimental data. Line is a guide for the eye.